

Atomistic Studies of PBX-9501 Constituents and Interactions Among Them

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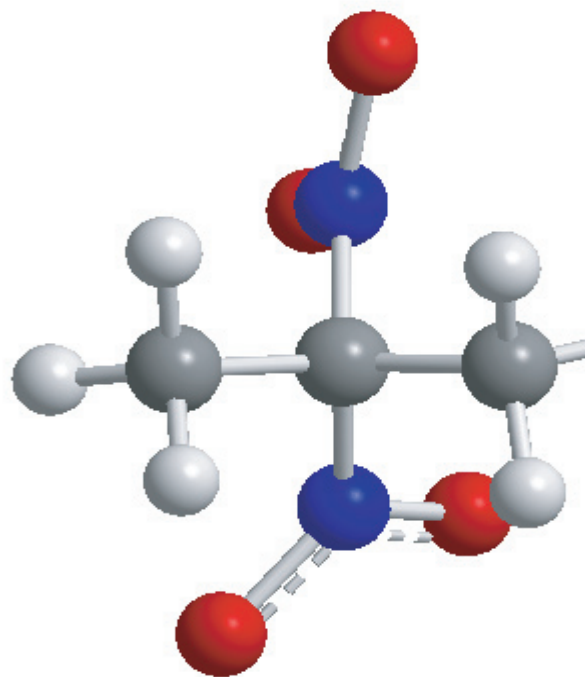
We are performing a variety of simulations designed to provide specific information or qualitative insights regarding the physical behaviors of the constituents of PBX-9501. The common thread among them is that they are based on calculations at the atomistic scale. The work is part of a larger effort to provide physically based continuum constitutive models for PBX-9501 on the basis of processes that occur at subcontinuum length scales. Our present work is a continuation of a research program that has been underway for several years and that involves close interactions between theorists working at atomistic and mesoscopic scales, as well as collaborations between theorists and experimentalists.

The zero Kelvin isotherm has been computed for β -HMX crystal in the pressure interval 0–10 GPa using the MondoSCF quantum chemistry code, at the PBE/6-31G** level of theory (Fig. 1). The zero Kelvin isotherm can serve as a reference curve for the construction of a P-V-T equation of state for a material at elevated temperatures. Whereas similar calculations for PETN yielded excellent agreement with experiment, the results for β -HMX reveal systematic discrepancies from data. Understanding this is an area of ongoing investigation.

In previous work, quantum-chemistry-based force fields were developed for HMX and Estane™. We are presently in the final stages of developing an analogous force field for bis(2,2-dinitropropyl) formal/acetal (BDNPF/A), which is the plasticizer in

the binder for PBX-9501 (Fig. 2). Upon completion of this force field, we will have a consistent, quantum-chemistry-based potential function for all of the major constituents of PBX-9501. This will enable us to study detailed physical interactions in that material; for example, the nature of the high-explosive/binder interface and the influence of plasticization on the properties of the binder.

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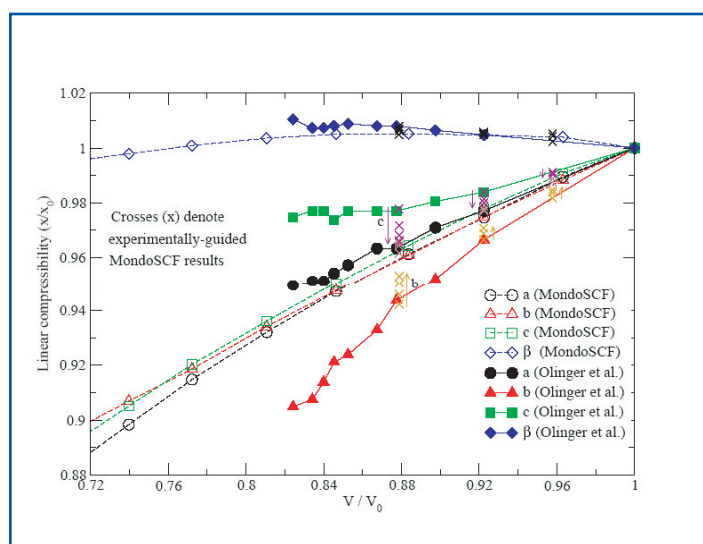


Figure 1—
Linear compressibilities
for β -HMX.

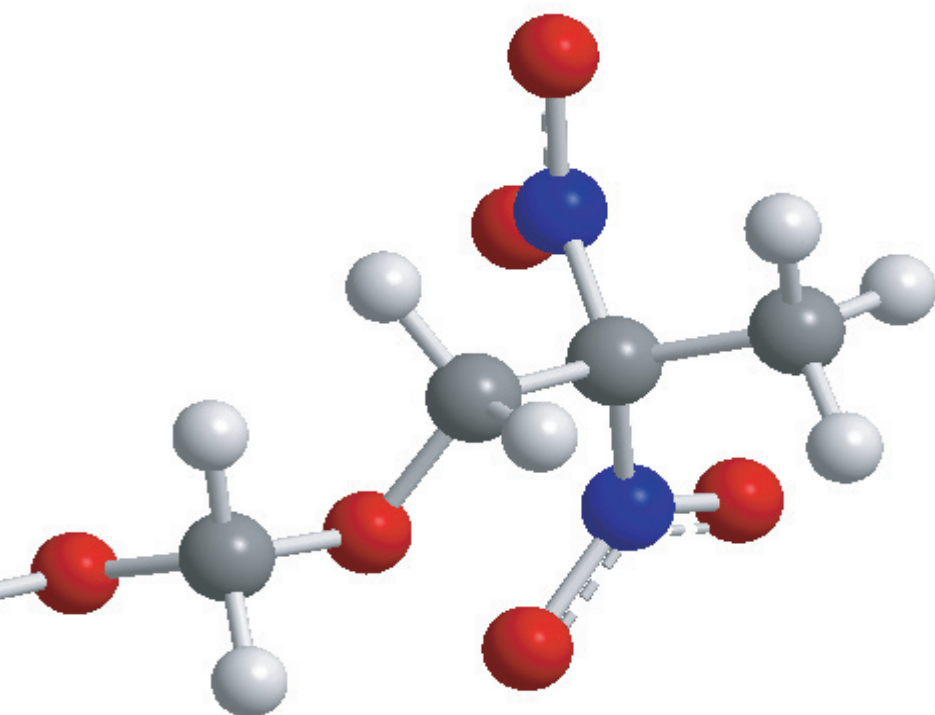


Figure 2—
Chemical structure of
BDNPF plasticizer.